4-Methylindan

824-22-6 | DTXSID7073931

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		**Training (75%)**		**Test (25%)**	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.06e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.28e-01

Confidence level: 6.16e-01

Nearest Neighbors from the Training Set

Image not found
5-Ethylidene-2-norbornene
Measured: 7.40e-05
Predicted: 2.32e-04

Image not found
Terpinolene
Measured: 6.97e-05
Predicted: 6.64e-05

Image not found
Lindane
Measured: 9.42e-06
Predicted: 6.40e-06

Image not found
alpha-1,2,3,4,5,6-Hexachlorocyclohexane
Measured: 9.42e-06
Predicted: 6.40e-06

Image not found
beta-Hexachlorocyclohexane
Measured: 9.42e-06
Predicted: 6.40e-06

Image not found
delta-Hexachlorocyclohexane
Measured: 9.42e-06
Predicted: 6.40e-06

Image not found
1,2,3,4,5,6-Hexachlorocyclohexane
Measured: 9.42e-06
Predicted: 6.40e-06

Image not found
Bromocyclohexane
Measured: 5.08e-03
Predicted: 2.15e-03

Image not found
1-Heptanethiol
Measured: 7.00e-05
Predicted: 6.62e-05